

1,1,2,3,3,3-Hexafluoro-1-propene
116-15-4 | DTXSID2026949

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -149 °C

Global applicability domain: Outside

Local applicability domain index: 5.41e-01

Confidence level: 6.88e-01

Nearest Neighbors from the Training Set

Image not found

1,1,2,3,3,3-Hexafluoro-1-propene

Measured: -157

Predicted: -149

Image not found

2-Butene, 1,1,1,2,3,4,4,4-octafluoro-

Measured: -129

Predicted: -121

Image not found

Tetrafluoroethylene

Measured: -143

Predicted: -139

Image not found

2-Butyne, 1,1,1,4,4,4-hexafluoro-

Measured: -117

Predicted: -109

Image not found

Hexafluoro-1,3-butadiene

Measured: -132

Predicted: -120